

# 4-Oxapyrene-5-one

<b>Inchi:</b>	InChI=1S/C15H8O2/c16-15-11-5-1-3-9-7-8-10-4-2-6-12(17-15)14(10)13(9)11/h1-8H
<b>InchiKey:</b>	SJXDHZGVKPNCHK-UHFFFAOYSA-N
<b>Formula:</b>	C15H8O2
<b>SMILES:</b>	O=c1oc2cccc3ccc4cccc1c4c32
<b>Mol. weight [g/mol]:</b>	220.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.46		Crippen Method
logp	3.537		Crippen Method
mcvol	156.110	ml/mol	McGowan Method
rinpol	375.60		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R287788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R287788&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/91-250-3/4-Oxapyrene-5-one.pdf>

Generated by Cheméo on 2024-04-20 09:39:55.961133229 +0000 UTC m=+15895244.881710541.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.